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Supplementary Material

Tuning the adsorption behavior of *β*-structure chitosan by metal binding

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Text S1 Three isotherm equations

The Langmuir isotherm was originally proposed to describe the adsorption of gas molecules onto metal surfaces. The model assumes uniform energy of the adsorption onto the surface and no migration of the adsorbate in the plane of the surface. It is expressed as

$$q_e = \frac{q_m K_L C_e}{1 + K_L C_e} \tag{1}$$

where q_e is the amount of pollutant adsorbed at equilibrium (mg/g) and C_e is the adsorbate concentration at equilibrium in aqueous solution (mg/L). The Langmuir isotherm parameters are q_m and K_L. The capacity of the adsorbent can be evaluated by q_m, and the parameter K_L includes various physical constants.

The Freundlich isotherm describes heterogeneous systems as the surfaces with nonenergetically equivalent sites. The equation can be written as follows:

$$q_e = K_f C_e^{1/n} \tag{2}$$

where K_f is the Freundlich constant, which is indicative of the extent of adsorption, and $1/n$ is the heterogeneity factor, an indicator of adsorption effectiveness. Another useful equation is the Langmuir-Freundlich isotherm, which is based on the generalized Langmuir and generalized exponential isotherms and is the most promising extension of the Langmuir and Freundlich isotherms. It is expressed as

$$q_e = \frac{q_m (K_{lf} C_e)^v}{1 + (K_{lf} C_e)^v} \tag{3}$$

where q_m is the maximum adsorption (mg/g), K_{lf} is the Langmuir-Freundlich constant, and v is the Langmuir-Freundlich heterogeneity constant. The Langmuir-Freundlich isotherm is essentially the Freundlich isotherm approaching a maximum at high concentrations.

Table S1 Parameters of Langmuir-Freundlich isotherm models for AR 73, Cr(VI) and F^- adsorption on chitosan based adsorbents.

Adsorbents	Equation	Pollutants	Parameters	R^2
***α*-CS**	$q_e = \frac{q_m(K_{lf}C_e)^v}{1+(K_{lf}C_e)^v}$	AR 73	q_m = 247.45 mg/g, K_{lf} = 0.0020 (L/mg)$^{1/v}$, v = 0.6448	0.9877
		Cr(VI)	q_m = 233.02 mg/g, K_{lf} = 0.0001 (L/mg)$^{1/v}$, v = 0.5573	0.9935
		F^-	/	/
***β*-CS**		AR 73	q_m = 223.12 mg/g, K_{lf} = 0.0010 (L/mg)$^{1/v}$, v = 0.7508	0.9866
		Cr(VI)	q_m = 157.01 mg/g, K_{lf} = 0.0003 (L/mg)$^{1/v}$, v = 0.5034	0.9835
		F^-	/	/
***α*-CS-Fe**		AR 73	q_m = 302.48 mg/g, K_{lf} = 0.1266 (L/mg)$^{1/v}$, v = 0.4628	0.9898
		Cr(VI)	q_m = 131.76 mg/g, K_{lf} = 0.0089 (L/mg)$^{1/v}$, v = 0.4450	0.9824
		F^-	q_m = 60.80 mg/g K_{lf} = 0.0056 (L/mg)$^{1/v}$, v = 0.9849	0.9982
***β*-CS-Fe**		AR 73	q_m = 501.86 mg/g, K_{lf} = 0.8670 (L/mg)$^{1/v}$, v = 0.3894	0.9679
		Cr(VI)	q_m = 176.66 mg/g, K_{lf} = 30.09 (L/mg)$^{1/v}$, v = 0.4590	0.9830
		F^-	q_m = 108.10 mg/g K_{lf} = 0.0040 (L/mg)$^{1/v}$, v = 1.44	0.9742
***α*-CS-Fe-Al**		AR 73	q_m = 420.53 mg/g, K_{lf} = 0.5248 (L/mg)$^{1/v}$, v = 0.6448	0.9284
		Cr(VI)	q_m = 130.25 mg/g, K_{lf} = 0.6737 (L/mg)$^{1/v}$, v = 0.2743	0.9338
		F^-	q_m = 124.24 mg/g K_{lf} = 0.0052 (L/mg)$^{1/v}$, v = 0.7716	0.9988
***β*-CS-Fe-Al**		AR 73	q_m = 621.45 mg/g, K_{lf} = 0.5248 (L/mg)$^{1/v}$, v = 0.6448	0.9692
		Cr(VI)	q_m = 173.03 mg/g, K_{lf} = 0.2916 (L/mg)$^{1/v}$, v = 0.2614	0.9536
		F^-	q_m = 144.53 mg/g K_{lf} = 0.0151 (L/mg)$^{1/v}$, v = 0.5901	0.9969

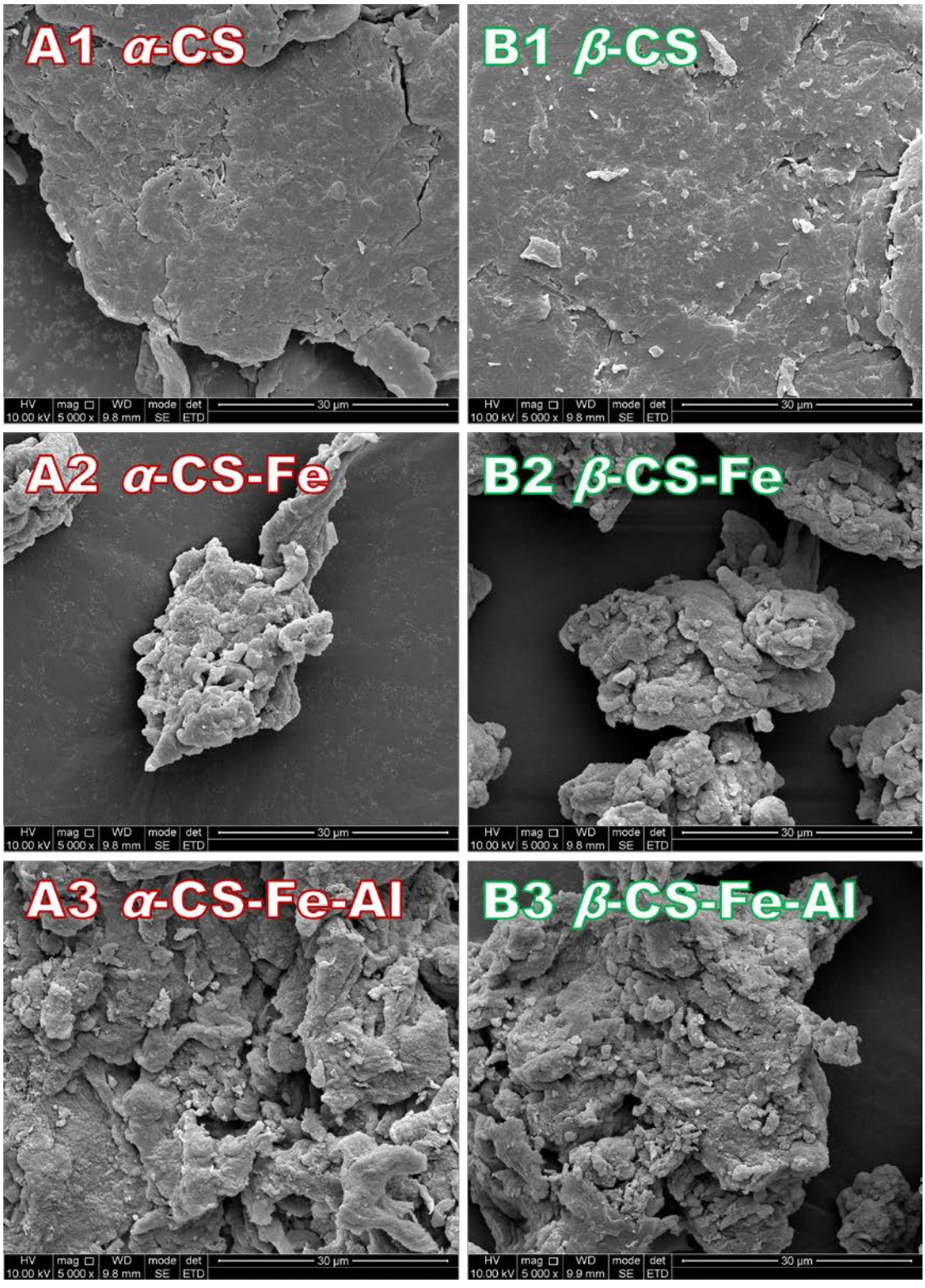

Figure S1 The SEM images of chitosan-metal complex with lower magnification

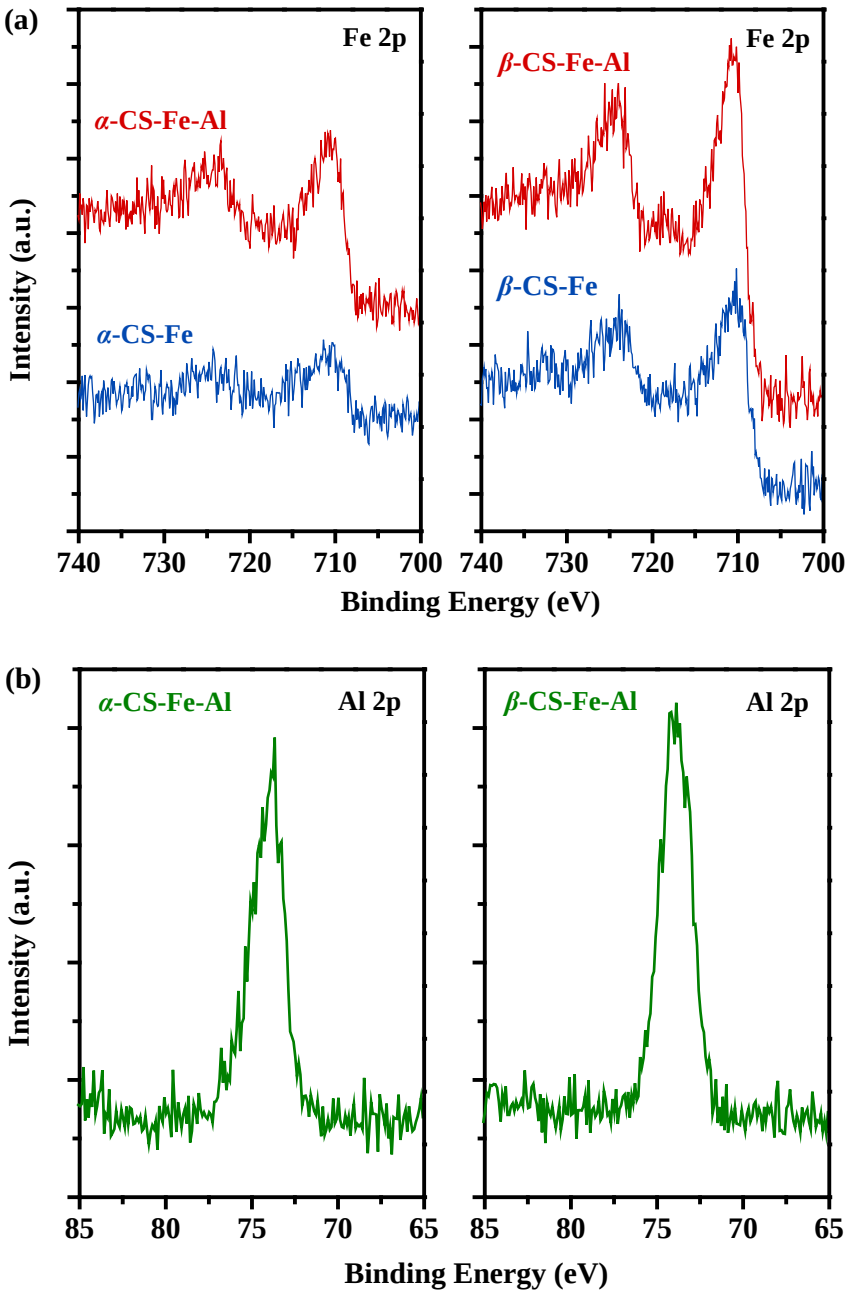

Figure S2 (a) Fe 2p and (b) Al 2p XPS spectra of *α*- and *β*-structure chitosan-metal complexes.